Abstract

A method for selecting a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDKI) is provided. The method may comprise modelling a three dimensional structure of a plurality of molecules in a computer, comparing with the three dimensional structure of the compounds with that of a reference structure such as at least part of a protein kinase catalytic domain of PDK1, and selecting the compound based on a predicted interacting ability of the molecules to the protein kinase catalytic domain. Also a method for selecting a compound for modulating the activity of hydrophobic pocket containing protein kinase is provided. In this method, the reference structures may be one or more of a phosphate binding pocket of PDK1, a hydrophobic pocket of PDK1, and αC helix or region interacting therewith of PDK1.